



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:54 AM GMT

PDB ID : 3Q9K  
Title : Crystal structure of bovine lactoperoxidase complexed with Phenyl isothiocyanate at 1.7 Å resolution  
Authors : Pandey, N.; Singh, A.K.; Singh, R.P.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2011-01-08  
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

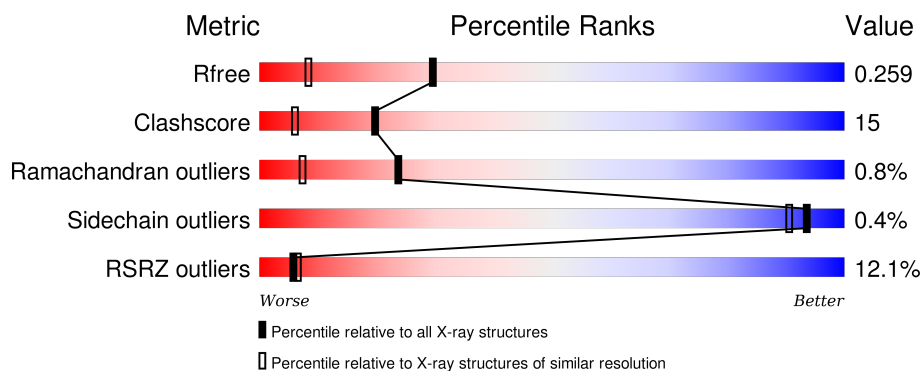
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	595	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	FTE	A	598	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PEG	A	610	-	-	X	X
11	PEG	A	613	-	-	X	X
12	MPD	A	615	-	-	X	X
5	NAG	A	601	-	-	-	X
8	GOL	A	597	-	-	-	X
9	SCN	A	700	-	X	-	-

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 5629 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4774	3037	847	863	1	26			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total	I	0	0
			12	12		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

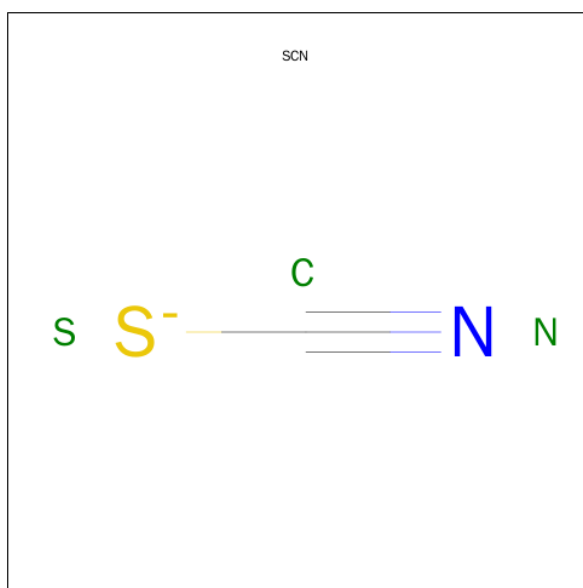
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



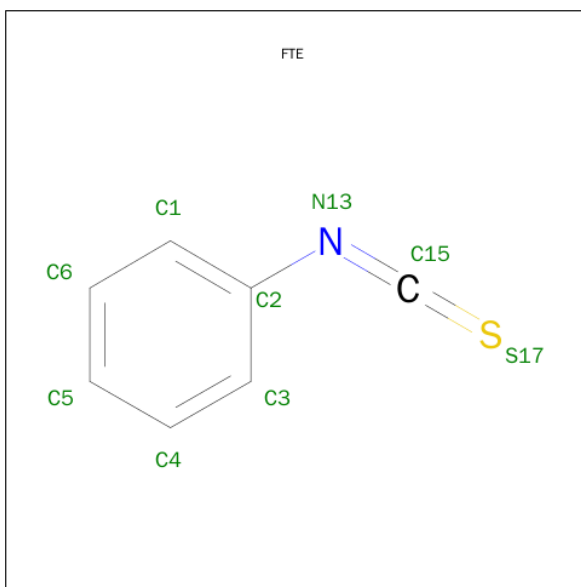
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is THIOCYANATE ION (three-letter code: SCN) (formula:  $CNS$ ).



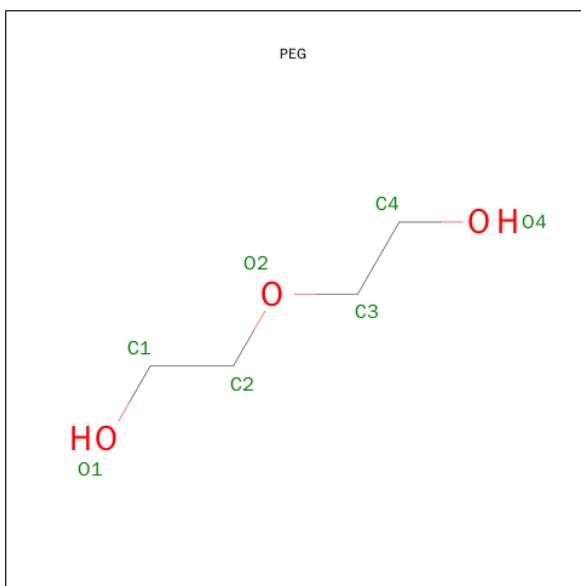
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 10 is PHENYLISOTHIOCYANATE (three-letter code: FTE) (formula:  $C_7H_5NS$ ).



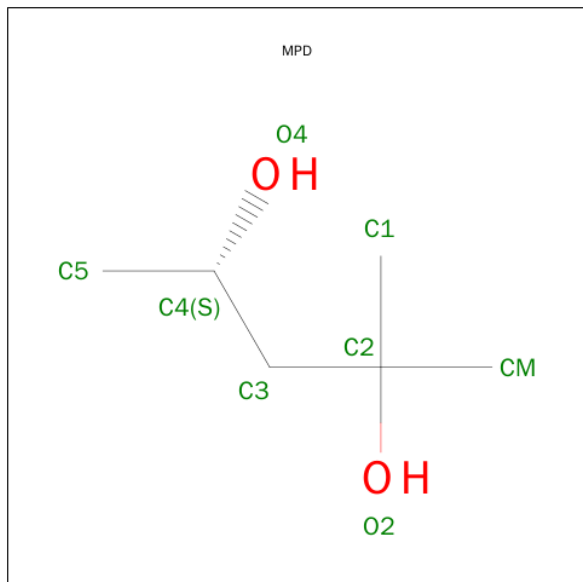
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	S	0	0
			9	7	1	1		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



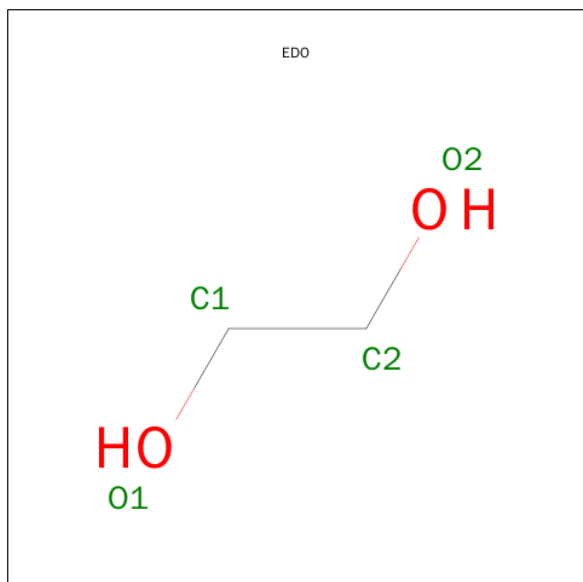
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			7	4	3		
11	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 12 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 13 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			4	2	2		

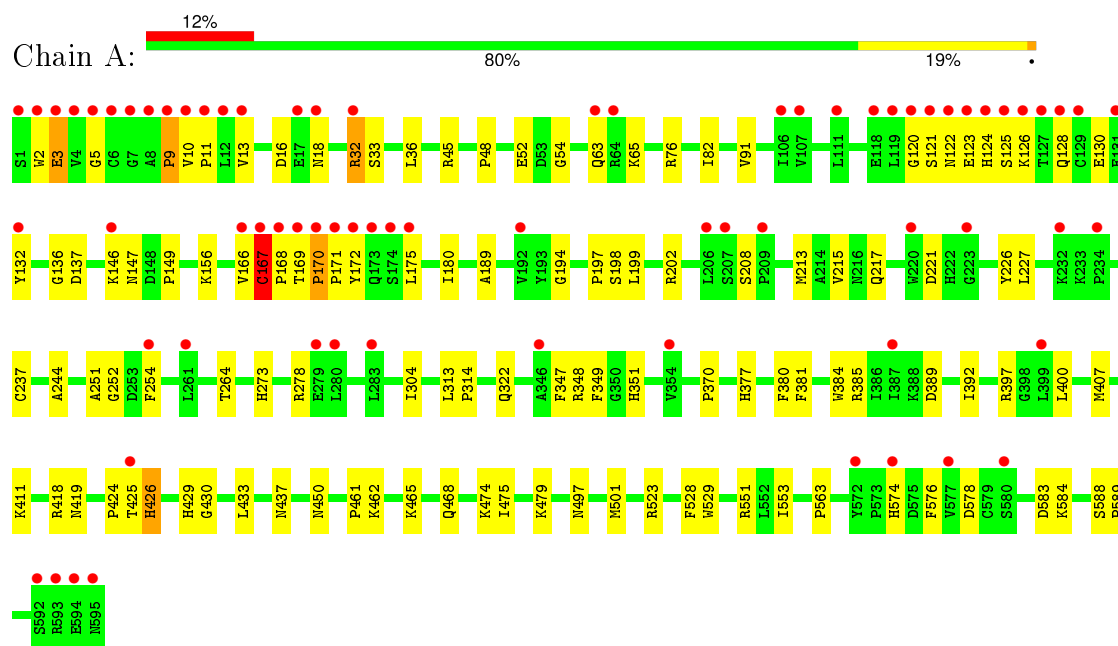
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	680	Total	O	0	0
			680	680		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: lactoperoxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.91Å 79.69Å 76.97Å 90.00° 102.24° 90.00°	Depositor
Resolution (Å)	23.60 – 1.70 39.41 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.9 (23.60-1.70) 97.6 (39.41-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.222 , 0.236 0.217 , 0.259	Depositor DCC
$R_{free}$ test set	3506 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	5 of 68803 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, SCN, NAG, SEP, CA, MPD, EDO, FTE, HEM, PEG, IOD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.73	1/4891 (0.0%)	0.83	2/6634 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	CYS	CB-SG	-6.41	1.71	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	GLU	N-CA-C	5.53	125.94	111.00
1	A	426	HIS	N-CA-C	-5.38	96.48	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4687	138	0
2	A	1	0	0	0	0
3	A	43	0	30	2	0
4	A	42	0	39	2	0
5	A	28	0	25	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	12	0	0	2	0
7	A	1	0	0	0	0
8	A	6	0	8	2	0
9	A	3	0	0	0	0
10	A	9	0	5	2	0
11	A	14	0	18	9	0
12	A	8	0	12	11	0
13	A	8	0	10	2	0
14	A	680	0	0	34	0
All	All	5629	0	4834	146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLY:HA2	1:A:123:GLU:HG2	1.46	0.98
1:A:82:ILE:HD11	1:A:479:LYS:HB3	1.45	0.98
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.48	0.94
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.50	0.93
1:A:462:LYS:HD2	14:A:1097:HOH:O	1.68	0.93
1:A:120:GLY:HA2	1:A:123:GLU:CG	1.99	0.92
1:A:32:ARG:HH11	1:A:32:ARG:CG	1.82	0.91
1:A:278:ARG:HD2	14:A:660:HOH:O	1.70	0.89
1:A:32:ARG:HH11	1:A:32:ARG:HG3	1.38	0.88
1:A:202:ARG:HD3	12:A:615:MPD:HM1	1.55	0.87
1:A:199:LEU:HB2	12:A:615:MPD:H11	1.57	0.85
6:A:614:IOD:I	14:A:1060:HOH:O	2.67	0.81
1:A:48:PRO:HD3	11:A:613:PEG:H42	1.62	0.80
1:A:126:LYS:HE3	1:A:425:THR:HG21	1.65	0.78
1:A:82:ILE:HD11	1:A:479:LYS:CB	2.12	0.78
5:A:602:NAG:H61	14:A:924:HOH:O	1.86	0.76
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.15	0.75
1:A:121:SER:C	1:A:122:ASN:HD22	1.91	0.74
1:A:120:GLY:HA2	1:A:123:GLU:CD	2.08	0.73
1:A:48:PRO:HA	11:A:613:PEG:H12	1.69	0.73
1:A:120:GLY:HA2	1:A:123:GLU:OE1	1.88	0.73
11:A:613:PEG:H11	14:A:727:HOH:O	1.87	0.73
1:A:146:LYS:HE3	14:A:1303:HOH:O	1.88	0.73
1:A:166:VAL:O	1:A:168:PRO:HD2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PRO:HG3	1:A:172:TYR:CG	2.25	0.71
1:A:197:PRO:HD2	1:A:198:SEP:O2P	1.92	0.70
1:A:123:GLU:CD	1:A:125:SER:OG	2.30	0.70
1:A:32:ARG:NH1	1:A:32:ARG:HG3	2.06	0.69
1:A:130:GLU:OE1	1:A:426:HIS:ND1	2.26	0.66
1:A:13:VAL:HG12	14:A:937:HOH:O	1.95	0.65
1:A:407:MET:HB3	1:A:501:MET:HE3	1.78	0.64
1:A:202:ARG:HD3	12:A:615:MPD:CM	2.28	0.64
1:A:124:HIS:HD2	14:A:1245:HOH:O	1.80	0.64
1:A:132:TYR:HE1	14:A:729:HOH:O	1.79	0.63
1:A:45:ARG:HB2	11:A:613:PEG:H21	1.79	0.63
1:A:54:GLY:HA2	14:A:945:HOH:O	1.98	0.63
1:A:82:ILE:CD1	1:A:479:LYS:HB3	2.24	0.63
1:A:36:LEU:HD11	8:A:597:GOL:H2	1.81	0.63
1:A:588:SER:HB2	14:A:1249:HOH:O	1.99	0.63
1:A:120:GLY:CA	1:A:123:GLU:HG2	2.27	0.62
1:A:168:PRO:HG3	1:A:172:TYR:HB2	1.81	0.62
1:A:254:PHE:CE2	10:A:598:FTE:H4	2.35	0.62
1:A:348:ARG:HH11	1:A:437:ASN:ND2	1.97	0.61
1:A:149:PRO:HG2	11:A:610:PEG:H22	1.80	0.61
1:A:63:GLN:CD	1:A:63:GLN:H	2.03	0.61
1:A:168:PRO:HG3	1:A:172:TYR:CB	2.31	0.61
1:A:202:ARG:HH11	12:A:615:MPD:HM1	1.65	0.60
1:A:407:MET:HB3	1:A:501:MET:CE	2.30	0.60
1:A:120:GLY:CA	1:A:123:GLU:OE1	2.48	0.60
1:A:91:VAL:HG12	1:A:411:LYS:HD3	1.83	0.60
1:A:10:VAL:HG11	14:A:1022:HOH:O	2.01	0.59
1:A:33:SER:HB3	1:A:36:LEU:HD12	1.85	0.59
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.50	0.59
1:A:418:ARG:HH22	11:A:610:PEG:H12	1.67	0.59
1:A:156:LYS:HD2	14:A:730:HOH:O	2.02	0.59
1:A:168:PRO:CG	1:A:172:TYR:HB2	2.33	0.58
1:A:124:HIS:CD2	14:A:1245:HOH:O	2.56	0.58
5:A:602:NAG:H62	14:A:874:HOH:O	2.04	0.56
1:A:450:ASN:OD1	1:A:461:PRO:HD2	2.05	0.56
1:A:244:ALA:HB2	5:A:601:NAG:H62	1.87	0.56
1:A:175:LEU:HD12	14:A:1168:HOH:O	2.05	0.55
1:A:199:LEU:CD1	12:A:615:MPD:HM2	2.37	0.55
1:A:381:PHE:CD2	1:A:381:PHE:N	2.75	0.55
1:A:122:ASN:HB3	14:A:1119:HOH:O	2.06	0.54
1:A:377:HIS:CD2	13:A:616:EDO:H11	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.42	0.54
1:A:13:VAL:HG13	14:A:956:HOH:O	2.07	0.54
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.90	0.54
1:A:322:GLN:HG2	14:A:755:HOH:O	2.07	0.53
3:A:605:HEM:HBD2	14:A:1093:HOH:O	2.09	0.53
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.43	0.53
1:A:167:CYS:CB	1:A:168:PRO:CD	2.86	0.52
1:A:418:ARG:NH2	11:A:610:PEG:H12	2.25	0.52
1:A:208:SER:CB	4:A:599:NAG:H62	2.39	0.52
1:A:166:VAL:HG12	1:A:180:ILE:HG12	1.90	0.52
1:A:170:PRO:HB2	1:A:171:PRO:CD	2.31	0.52
1:A:32:ARG:HH11	1:A:32:ARG:HG2	1.67	0.52
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.91	0.52
1:A:82:ILE:CD1	1:A:479:LYS:CB	2.85	0.51
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.93	0.50
1:A:121:SER:O	1:A:122:ASN:ND2	2.35	0.50
1:A:52:GLU:HG2	1:A:65:LYS:HD2	1.94	0.50
3:A:605:HEM:HMC2	3:A:605:HEM:HBC2	1.94	0.50
6:A:618:IOD:I	14:A:1064:HOH:O	2.89	0.50
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.94	0.49
1:A:45:ARG:CB	11:A:613:PEG:H21	2.43	0.49
1:A:2:TRP:HE3	1:A:3:GLU:OE1	1.96	0.49
1:A:424:PRO:O	1:A:425:THR:HB	2.12	0.49
1:A:123:GLU:HB3	14:A:1088:HOH:O	2.13	0.49
1:A:199:LEU:CB	12:A:615:MPD:H11	2.34	0.49
1:A:202:ARG:NH1	12:A:615:MPD:HM1	2.28	0.49
1:A:385:ARG:O	1:A:389:ASP:HB3	2.13	0.48
1:A:400:LEU:HD21	1:A:553:ILE:CD1	2.43	0.48
1:A:208:SER:HB3	4:A:599:NAG:H62	1.94	0.48
1:A:370:PRO:HD2	14:A:1013:HOH:O	2.12	0.48
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.95	0.47
1:A:3:GLU:HG2	14:A:1050:HOH:O	2.14	0.47
8:A:597:GOL:H12	14:A:1117:HOH:O	2.15	0.47
1:A:91:VAL:CG1	1:A:411:LYS:HD3	2.44	0.47
1:A:429:HIS:CE1	13:A:616:EDO:H22	2.49	0.47
1:A:199:LEU:HD12	12:A:615:MPD:HM2	1.96	0.47
1:A:227:LEU:CD2	1:A:251:ALA:HB2	2.45	0.47
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.33	0.46
1:A:465:LYS:NZ	14:A:681:HOH:O	2.45	0.46
1:A:18:ASN:ND2	14:A:943:HOH:O	2.48	0.46
1:A:419:ASN:O	1:A:430:GLY:HA2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:HG3	1:A:167:CYS:H	1.79	0.46
1:A:198:SEP:HB3	12:A:615:MPD:H52	1.97	0.46
1:A:121:SER:C	1:A:122:ASN:ND2	2.64	0.46
1:A:126:LYS:CE	1:A:425:THR:HG21	2.43	0.45
1:A:128:GLN:O	1:A:128:GLN:HG3	2.15	0.45
1:A:146:LYS:HZ2	1:A:147:ASN:HD21	1.64	0.45
1:A:128:GLN:HB2	14:A:1245:HOH:O	2.17	0.44
1:A:76:ARG:HH22	11:A:610:PEG:H11	1.81	0.44
1:A:424:PRO:C	1:A:426:HIS:H	2.19	0.44
1:A:588:SER:CB	14:A:1249:HOH:O	2.63	0.44
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.53	0.44
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.53	0.44
1:A:551:ARG:HD3	1:A:583:ASP:O	2.18	0.44
1:A:202:ARG:CD	12:A:615:MPD:HM1	2.38	0.44
1:A:3:GLU:HG3	1:A:5:GLY:HA2	1.99	0.43
1:A:578:ASP:OD1	14:A:1150:HOH:O	2.21	0.43
1:A:574:HIS:HD2	14:A:1151:HOH:O	2.00	0.43
1:A:381:PHE:HE1	10:A:598:FTE:C6	2.31	0.43
1:A:13:VAL:CG1	14:A:956:HOH:O	2.64	0.43
1:A:237:CYS:HA	1:A:381:PHE:O	2.18	0.43
1:A:397:ARG:NH2	14:A:899:HOH:O	2.51	0.43
1:A:264:THR:HG23	1:A:392:ILE:HB	2.01	0.43
1:A:16:ASP:OD1	1:A:16:ASP:C	2.57	0.42
1:A:227:LEU:HD23	1:A:251:ALA:HB2	2.02	0.42
1:A:199:LEU:HD13	12:A:615:MPD:HM2	2.00	0.42
1:A:146:LYS:NZ	1:A:147:ASN:HD21	2.17	0.42
1:A:215:VAL:HG23	1:A:217:GLN:NE2	2.35	0.42
1:A:313:LEU:N	1:A:314:PRO:CD	2.82	0.41
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.34	0.41
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.56	0.41
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.34	0.41
1:A:221:ASP:HB2	1:A:226:TYR:CE2	2.56	0.41
1:A:82:ILE:HD13	1:A:479:LYS:HD3	2.03	0.41
1:A:136:GLY:O	1:A:137:ASP:HB2	2.21	0.41
1:A:528:PHE:O	1:A:529:TRP:C	2.58	0.41
1:A:384:TRP:CZ2	5:A:601:NAG:H2	2.56	0.41
1:A:425:THR:O	1:A:425:THR:HG22	2.20	0.40
1:A:475:ILE:HG13	14:A:767:HOH:O	2.22	0.40
1:A:194:GLY:HA2	1:A:252:GLY:O	2.21	0.40
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.56	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	592/595 (100%)	558 (94%)	29 (5%)	5 (1%)	24 7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	11	PRO
1	A	167	CYS
1	A	170	PRO
1	A	169	THR

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	517/517 (100%)	515 (100%)	2 (0%)	93 90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	347	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	147	ASN
1	A	217	GLN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	570	ASN
1	A	595	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEP	A	198	1	8,9,10	1.84	3 (37%)	8,12,14	3.94	3 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	198	1	-	0/6/8/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	-3.72	1.38	1.51
1	A	198	SEP	P-O2P	-2.07	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	CA-N	-2.06	1.41	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O3P-P-O1P	-2.63	102.11	110.58
1	A	198	SEP	OG-P-O1P	6.76	124.35	107.14
1	A	198	SEP	OG-CB-CA	8.28	115.34	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	2	0

## 5.5 Carbohydrates ⓘ

2 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	601	1,5	14,14,15	0.95	1 (7%)	15,19,21	1.07	2 (13%)
5	NAG	A	602	5	14,14,15	0.69	0	15,19,21	2.24	7 (46%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	602	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	NAG	O5-C1	-2.24	1.40	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	NAG	C4-C3-C2	-3.24	106.19	111.23
5	A	602	NAG	O3-C3-C4	-2.79	104.05	110.34
5	A	602	NAG	O7-C7-C8	-2.62	117.26	122.06
5	A	601	NAG	C1-O5-C5	-2.49	109.09	112.25
5	A	601	NAG	C2-N2-C7	-2.12	120.31	123.04
5	A	602	NAG	C3-C2-N2	2.13	115.67	110.56
5	A	602	NAG	O5-C5-C6	2.56	112.90	107.35
5	A	602	NAG	C3-C4-C5	2.72	114.94	110.20
5	A	602	NAG	C1-O5-C5	5.00	118.60	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	NAG	2	0
5	A	602	NAG	2	0

## 5.6 Ligand geometry

Of 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	596	1	14,14,15	0.71	0	15,19,21	1.18	2 (13%)
8	GOL	A	597	-	5,5,5	0.45	0	5,5,5	0.26	0
10	FTE	A	598	-	6,9,9	0.64	0	8,10,10	0.31	0
4	NAG	A	599	1	14,14,15	0.65	0	15,19,21	1.22	3 (20%)
4	NAG	A	604	1	14,14,15	0.41	0	15,19,21	1.16	2 (13%)
3	HEM	A	605	1	30,50,50	2.64	7 (23%)	24,82,82	2.25	6 (25%)
11	PEG	A	610	-	6,6,6	0.93	0	5,5,5	0.57	0
11	PEG	A	613	-	6,6,6	0.97	0	5,5,5	0.27	0
12	MPD	A	615	-	6,7,7	2.70	3 (50%)	7,10,10	1.13	0
13	EDO	A	616	-	3,3,3	1.35	1 (33%)	2,2,2	0.45	0
13	EDO	A	617	-	3,3,3	1.00	0	2,2,2	0.13	0
9	SCN	A	700	-	2,2,2	2.46	1 (50%)	1,1,1	3.58	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	596	1	-	0/6/23/26	0/1/1/1
8	GOL	A	597	-	-	0/4/4/4	0/0/0/0
10	FTE	A	598	-	-	0/0/3/3	0/1/1/1
4	NAG	A	599	1	-	0/6/23/26	0/1/1/1
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
3	HEM	A	605	1	-	0/10/54/54	0/0/8/8
11	PEG	A	610	-	-	0/4/4/4	0/0/0/0
11	PEG	A	613	-	-	0/4/4/4	0/0/0/0
12	MPD	A	615	-	-	0/5/5/5	0/0/0/0
13	EDO	A	616	-	-	0/1/1/1	0/0/0/0
13	EDO	A	617	-	-	0/1/1/1	0/0/0/0
9	SCN	A	700	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	HEM	C3B-C4B	-10.36	1.42	1.51
12	A	615	MPD	O2-C2	-5.20	1.30	1.44
3	A	605	HEM	C3D-C4D	-5.10	1.45	1.51
3	A	605	HEM	C2C-C1C	-4.96	1.43	1.52
12	A	615	MPD	O4-C4	-2.54	1.30	1.43
3	A	605	HEM	C2B-C1B	-2.20	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	616	EDO	O2-C2	-2.19	1.30	1.42
12	A	615	MPD	C5-C4	-2.19	1.42	1.51
3	A	605	HEM	C3C-CAC	2.63	1.56	1.51
3	A	605	HEM	C4C-NC	2.64	1.39	1.36
9	A	700	SCN	C-S	3.17	1.84	1.63
3	A	605	HEM	C3B-CAB	3.17	1.57	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	700	SCN	S-C-N	-3.58	151.77	175.94
3	A	605	HEM	CAA-C2A-C1A	-3.26	123.47	127.01
4	A	604	NAG	C2-N2-C7	-3.11	119.05	123.04
4	A	596	NAG	C4-C3-C2	-2.52	107.31	111.23
4	A	599	NAG	C3-C2-N2	-2.38	104.87	110.56
3	A	605	HEM	CAA-CBA-CGA	-2.29	108.55	112.75
4	A	604	NAG	C4-C3-C2	-2.26	107.71	111.23
4	A	599	NAG	C1-O5-C5	-2.19	109.47	112.25
4	A	596	NAG	C2-N2-C7	-2.11	120.32	123.04
4	A	599	NAG	O4-C4-C3	-2.11	105.60	110.34
3	A	605	HEM	CMC-C2C-C3C	3.86	126.16	116.53
3	A	605	HEM	CAD-C3D-C2D	4.20	125.28	113.22
3	A	605	HEM	CMB-C2B-C3B	4.58	127.97	116.53
3	A	605	HEM	CAD-C3D-C4D	5.54	132.01	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	597	GOL	2	0
10	A	598	FTE	2	0
4	A	599	NAG	2	0
3	A	605	HEM	2	0
11	A	610	PEG	4	0
11	A	613	PEG	5	0
12	A	615	MPD	11	0
13	A	616	EDO	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	594/595 (99%)	1.02	72 (12%) 6 6	17, 30, 74, 100	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	GLY	21.8
1	A	2	TRP	18.1
1	A	4	VAL	16.1
1	A	172	TYR	13.8
1	A	124	HIS	13.3
1	A	121	SER	13.2
1	A	119	LEU	12.6
1	A	120	GLY	12.3
1	A	122	ASN	11.8
1	A	10	VAL	11.7
1	A	13	VAL	11.6
1	A	173	GLN	9.6
1	A	595	ASN	9.1
1	A	125	SER	8.9
1	A	8	ALA	8.9
1	A	593	ARG	8.1
1	A	123	GLU	7.9
1	A	171	PRO	7.6
1	A	6	CYS	7.6
1	A	170	PRO	7.5
1	A	11	PRO	7.1
1	A	174	SER	7.0
1	A	12	LEU	6.9
1	A	283	LEU	6.3
1	A	9	PRO	6.2
1	A	169	THR	5.5
1	A	209	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	18	ASN	5.2
1	A	132	TYR	5.1
1	A	594	GLU	5.0
1	A	3	GLU	4.9
1	A	1	SER	4.8
1	A	118	GLU	4.5
1	A	128	GLN	4.4
1	A	254	PHE	4.3
1	A	126	LYS	4.2
1	A	234	PRO	4.2
1	A	572	TYR	4.0
1	A	220	TRP	3.9
1	A	127	THR	3.7
1	A	129	CYS	3.7
1	A	166	VAL	3.6
1	A	64	ARG	3.5
1	A	17	GLU	3.4
1	A	223	GLY	3.4
1	A	280	LEU	3.3
1	A	425	THR	3.3
1	A	175	LEU	3.1
1	A	580	SER	3.0
1	A	167	CYS	2.9
1	A	106	ILE	2.8
1	A	346	ALA	2.8
1	A	232	LYS	2.7
1	A	354	VAL	2.7
1	A	111	LEU	2.7
1	A	168	PRO	2.6
1	A	5	GLY	2.6
1	A	32	ARG	2.6
1	A	146	LYS	2.4
1	A	63	GLN	2.4
1	A	131	GLU	2.3
1	A	574	HIS	2.3
1	A	207	SER	2.3
1	A	279	GLU	2.3
1	A	192	VAL	2.2
1	A	387	ILE	2.2
1	A	577	VAL	2.2
1	A	592	SER	2.2
1	A	206	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	261	LEU	2.1
1	A	107	VAL	2.0
1	A	399	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	A	198	10/11	0.86	0.19	-	30,42,44,44	0

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	A	601	14/15	0.79	0.20	2.20	61,64,68,72	0
5	NAG	A	602	14/15	0.77	0.32	-	51,58,61,61	0

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	PEG	A	610	7/7	0.88	0.22	10.24	23,28,33,34	0
12	MPD	A	615	8/8	0.92	0.31	9.24	10,30,38,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	FTE	A	598	9/9	0.81	0.41	6.14	18,18,18,18	9
11	PEG	A	613	7/7	0.85	0.15	3.34	32,34,36,36	0
8	GOL	A	597	6/6	0.84	0.30	3.14	25,27,37,38	0
3	HEM	A	605	43/43	0.97	0.17	1.12	17,19,22,26	0
4	NAG	A	599	14/15	0.74	0.16	0.51	66,68,72,80	0
9	SCN	A	700	3/3	0.93	0.15	-0.19	44,44,44,45	0
13	EDO	A	617	4/4	0.91	0.11	-0.20	33,39,39,41	0
6	IOD	A	623	1/1	0.97	0.08	-0.81	42,42,42,42	1
6	IOD	A	629	1/1	0.97	0.08	-1.68	34,34,34,34	1
6	IOD	A	622	1/1	0.95	0.04	-1.70	46,46,46,46	1
2	CA	A	606	1/1	0.99	0.12	-1.79	20,20,20,20	0
6	IOD	A	612	1/1	0.94	0.06	-2.46	46,46,46,46	0
6	IOD	A	621	1/1	0.92	0.05	-3.09	49,49,49,49	1
6	IOD	A	608	1/1	0.97	0.03	-3.27	35,35,35,35	0
6	IOD	A	607	1/1	1.00	0.02	-4.39	22,22,22,22	0
6	IOD	A	611	1/1	0.98	0.03	-6.53	31,31,31,31	0
4	NAG	A	604	14/15	0.79	0.26	-	49,53,59,60	0
6	IOD	A	618	1/1	0.91	0.07	-	57,57,57,57	1
6	IOD	A	614	1/1	0.97	0.05	-	40,40,40,40	1
13	EDO	A	616	4/4	0.91	0.14	-	29,34,37,37	0
7	ZN	A	630	1/1	0.97	0.03	-	40,40,40,40	0
4	NAG	A	596	14/15	0.51	0.37	-	62,66,69,69	0
6	IOD	A	620	1/1	0.94	0.04	-	50,50,50,50	1
6	IOD	A	609	1/1	0.93	0.07	-	51,51,51,51	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.